On the properties of the Uehling potential

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Abstract

A number of properties of the Uehling potential are investigated. In particular, we determine the Fourier spatial resolution of the Uehling potential. The lowest-order correction on vacuum polarisation is re-written in terms of the electron density distribution function. We also discuss the consecutive approximations of the perturbation theory developed for the short-range Uehling potential in the Coulomb few-body systems (atoms). The cusp problem is formulated for few-body systems in which particles interact with each other by the mixed (Coulomb + Uehling) potential.

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I. INTRODUCTION

As is well known (see, e.g., [1], [2]) in the lowest order approximation the effect of vacuum polarisation between two interacting electric charges is described by the Uehling potential $U(r)$ [3]. In [4] we have derived the closed analytical formula for the Uehling potential. For atomic systems this formula is written in the following three-term form (in atomic units $\hbar = 1, m_e = 1, e = 1$)

$$U(2br) = \frac{2\alpha Q}{3\pi} \cdot \frac{1}{r} \Big[\int_1^{+\infty} exp(-2\alpha^{-1}\xi r)\Big(1 + \frac{1}{2\xi^2}\Big)\frac{\sqrt{\xi^2 - 1}}{\xi^2} d\xi \Big]$$
$$= \frac{2\alpha Q}{3\pi r}\Big[\Big(1 + \frac{b^2 r^2}{3}\Big)K_0(2br) - \frac{br}{6}Ki_1(2br) - \Big(\frac{b^2 r^2}{3} + \frac{5}{6}\Big)Ki_2(2br)\Big] \quad , \tag{1}$$

where the notation Q stands for the electric charge of the nucleus, $b = \alpha^{-1}$ and $\alpha = \frac{e^2}{\hbar c} \approx \frac{1}{137}$ is the dimensionless fine-structure constant. Here and below $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant (also called the Dirac constant), e is the electric charge of the positron and m_e is the mass of the electron (= mass of the positron).

In Eq.(1) $K_0(a)$ is the modified Bessel function of zero order (see, e.g, [5]), i.e.

$$K_0(z) = \int_0^\infty exp(-z\cosh t)dt = \sum_{k=0}^\infty (\psi(k+1) + \ln 2 - \ln z)\frac{z^{2k}}{2^{2k}(k!)^2} \quad ,$$

where $\psi(k)$ is the Euler *psi*-function defined by Eq.(8.362) from [5]. The functions $Ki_1(z)$ and $Ki_2(z)$ in Eq.(1) are the recursive integrals of the $K_0(z) \equiv K_0(z)$ function, i.e.

$$Ki_1(z) = \int_z^\infty Ki_0(z)dz \quad , \quad and \quad Ki_n(z) = \int_z^\infty Ki_{n-1}(z)dz \quad , \tag{2}$$

where $n \geq 1$.

The closed analytical formula for the Uehling potential derived in [4] allows one to obtain substantial acceleration of numerical algorithms used to evaluate the effects of vacuum polarisation in various few-electron atoms and ions. On the other hand, the simple three-term formula, Eq.(1), can also be used to perform theoretical analysis of the vacuum polarisation itself. In this study we report some interesting results of our recent investigations. These results can be useful in numerical applications and may lead us to better understanding of vacuum polarisation in atomic systems. In particular, in this study we derive the general expression for the lowest-order correction on the vacuum polarisation in atoms and ions written with the use of the electron density distribution function $\rho(r)$. The arising expression has a number of advantages for theoretical analysis of vacuum polarisation in light atoms

and ions. Then we determine the spatial Fourier resolution of the Uehling potential $U(r)$. This leads us to the formula for the spatial Fourier resolution of the actual electrostatic field which is the sum of the regular Coulomb potential and short-range Uehling potential.

Another interesting problem is the application of the perturbation theory to determine various corrections produced by the short-range Uehling potential. It is shown in the fourth Section that all consecutive approximations produced by the Uehling potential can be determined with the use of the representations of the O(2,1)-algebra(s). Such an algebra describes the dynamical representations of the original Coulomb system (or atom). We also consider the cusp problem for few-body systems of interacting electrically charged particles.

II. UEHLING CORRECTION AND ELECTRON DENSITY DISTRIBUTION

In atomic systems the lowest-order correction on vacuum polarization $(\Delta E)_{V.P.}$ to the total energy of the $LS-$bound state is written in the following general form

$$(\Delta E)_{V.P.} = \int_0^\infty \Psi_{LS}^*(\mathbf{r})U(r)\Psi_{LS}(\mathbf{r})d^3\mathbf{r} = 4\pi \int_0^\infty \Psi_{LS}(r)U(r)\Psi_{LS}(r)r^2 dr$$
$$= 4\pi \int_0^\infty U(r)\rho_{LS}(r)r^2 dr \tag{3}$$

where $U(r)$ is the central Uehling potential Eq.(1). In Eq.(3) the notation $\Psi_{LS}(\mathbf{r})$ stands for the bound state wave function, while $\Psi_{LS}(r)$ means the radial part of the total wave function. The index LS designates the angular momentum and total (electron) spin of the bound state. We assume that the bound state wave function $\Psi_{LS}(r)$ is know. Furthermore, such a function can always be chosen as a real function (or it can be transformed into the real function). For the real wave function one finds $\Psi_{LS}^*(r) = \Psi_{LS}(r)$. The function $\rho(r) = \Psi_{LS}^*(r) \cdot \Psi_{LS}(r) = \Psi_{LS}(r) \cdot \Psi_{LS}(r)$ is the electron density distribution in the bound $LS-$atomic state. The formula which contains the electron density function $\rho(r)$ can also be applied in those cases when the atomic system occupies one of its 'mixed' states.

The expression for the $(\Delta E)_{V.P.}$, Eq.(3), can be transformed to the different form with the use of our formula from [4]. Indeed, we can write Eq.(3) as the sum of the three following terms T_1, T_2 and T_3, i.e.

$$(\Delta E)_{V.P.} = \frac{2\alpha Q}{3\pi}(T_1 + T_2 + T_3) \tag{4}$$

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The explicit expressions for the T_1, T_2 and T_3 terms are reduced to the form

$$T_1 = \frac{1}{4b^2} \int_0^\infty \left[1 + \frac{x^2}{12}\right] K_0(x) \rho(\frac{1}{2b}x) x dx \tag{5}$$

$$T_2 = -\frac{1}{48b^2} \int_0^\infty Ki_1(x) \rho(\frac{1}{2b}x) x^2 dx \tag{6}$$

$$T_3 = -\frac{1}{4b^2} \int_0^\infty Ki_2(x) \left(\frac{x^2}{12} + \frac{5}{6}\right) \rho(\frac{1}{2b}x) x dx \tag{7}$$

where $x = 2br$. The formulas for the T_2 and T_3 terms can be simplified by using a few different methods, e.g., integration by parts. Finally, the formula for the T_2 term takes the form

$$T_2 = -\frac{1}{48b^2} \int_0^\infty K_0(x) \Phi(x) dx = -\frac{1}{48b^2} \int_0^\infty K_0(x) \left[\int_0^x \rho(\frac{1}{2b}y) y^2 dy\right] dx \tag{8}$$

where the function $\Phi(x)$ is

$$\Phi(x) = \int_0^x \rho(\frac{1}{2b}y) y^2 dy \tag{9}$$

The term T_3 is transformed into a similar form

$$T_3 = -\frac{1}{48b^2} \int_0^\infty K_0(x) \Phi_1(x) dx = -\frac{1}{48b^2} \int_0^\infty K_0(x) \left[\int_0^x dz \int_0^z \left(\frac{y^3}{12} + \frac{5}{6}y\right) \rho(\frac{1}{2b}y) dy\right] dx \tag{10}$$

where the function $\Phi_1(x)$ is

$$\Phi_1(x) = \int_0^x dz \int_0^z \left[\frac{y^3}{12} + \frac{5}{6}y\right] \rho(\frac{1}{2b}y) dy \tag{11}$$

III.   FOURIER SPATIAL RESOLUTION OF THE UEHLING POTENTIAL

In various problems from atomic and molecular physics and Quantum Elecrodynamics it is often important to apply the correct analytical expression for the Fourier spectral resolution of the Uehling potential. It is clear *a priori* that the Uehling potential $U(r)$ is a static potential which also is a central potential. Therefore, we can expect that its representation as a superposition of plane waves will contain only plane waves of zero frequency. Moreover, it can be shown that such spatial waves are longitudinal, i.e. they are oriented along the spatial vector $\mathbf{k}$. The Fourier spatial resolution (or Fourier resolution, for short) of the Uehling potential is written in the form

$$U(\mathbf{r}) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} exp(\imath \mathbf{k} \cdot \mathbf{r}) u_{\mathbf{k}}(\mathbf{r}) \frac{d^3\mathbf{k}}{(2\pi)^3} \tag{12}$$

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where $\mathbf{k} = (k_x, k_y, k_z)$ is the wave vector and $u_{\mathbf{k}}(r)$ is the unknown spectral function. Our goal in this Section is to obtain the closed formula for this spectral function and compare it with the spectral function of the pure Coulomb potential.

From Eq.(12) one finds the following equation for the spectral function $u_{\mathbf{k}}(\mathbf{r}) = u_k(r)$

$$u(k) = \int \int \int U(r) exp(\imath \mathbf{k} \cdot \mathbf{r}) d^3 \mathbf{r} = 4\pi \int_0^{+\infty} j_0(kr) U(r) r^2 dr \tag{13}$$

where $k = \sqrt{k_x^2 + k_y^2 + k_z^2}$ is the radial component of the wave vector and $j_0(x)$ is the spherical Bessel function of zero order. Note also that the integration in the last formula is performed over the area occupied by the electric charges and electric field. In Eq.(13) we have used the fact that the Uehling potential is spherically symmetric and, therefore, we can integrate over all angular variables. By using Eq.(1) and expression for the $j_0(x) = \frac{sinx}{x}$ function one finds the following formula for the spectral function $u_k(r)$

$$u(k) = \frac{4\pi}{k} \int_1^{+\infty} \frac{1}{t^2 + a^2} \left(1 + \frac{1}{2t^2}\right) \frac{\sqrt{t^2 - 1}}{t^2} dt \tag{14}$$

where $a = \frac{k}{2b} = \frac{k\alpha}{2}$. The integral in the last equation can be determined with the use of the substitution $u = \frac{t}{\sqrt{t^2-1}}$. It reduces the integral to the form

$$I = \int_1^{+\infty} \frac{1}{t^2 + a^2} \left(1 + \frac{1}{2t^2}\right) \frac{\sqrt{t^2 - 1}}{t^2} dt = \frac{1}{2} \int_1^{+\infty} \frac{3u^2 - 1}{u^2(1 + a^2) - a^2} \cdot \frac{du}{u^4} \tag{15}$$

Then by using the substitution $y = \frac{1}{u}$ one transforms this integral to the form

$$I = \frac{1}{2a^2} \int_0^1 \frac{(3 - y^2)y^2 dy}{b^2 - y^2} = -\frac{5}{6a^2} + \frac{1}{2a^4} + \frac{2a^4 + a^2 - 1}{4a^6} ln(1 + 2a^2) \tag{16}$$

The final formula for the spatial spectral function takes the form

$$u(k) = \frac{2\pi}{k} \left[-\frac{5}{3a^2} + \frac{1}{a^4} + \frac{2a^4 + a^2 - 1}{2a^6} ln(1 + 2a^2)\right] \tag{17}$$

and, since $a = \frac{k\alpha}{2}$, we find

$$u(k) = \frac{4\pi}{k^3 \alpha^2} \left\{-\frac{10}{3} + \frac{8}{k^2 \alpha^2} + \frac{1}{k^4 \alpha^4} (k^4 \alpha^4 + 2k^2 \alpha^2 - 8) ln\left[1 + \frac{k^2 \alpha^2}{2}\right]\right\} \tag{18}$$

As follows from the last formula the first term in the expression for $u(k)$ is $\sim k^{-3}$. This gives the asymptotic of the spectral function at large wave numbers k. The analogous spectral function for the Coulomb potential between two interacting electrically charged particles is $u_C(k) = \frac{4\pi}{k^2}$ (in atomic units) (see, e.g., [6]). There are a number of differences between the

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two spectral functions $u(k)$, Eq.(18), and $u_C(r)$. First, the $u(r)$ function is an approximate cubic function upon k^{-1} (inverse wave number), while $u_C(k)$ is an exact quadratic function. Second, the $u(k)$ function, Eq.(18), contains inverse powers of the fine-structure constant α, while the $u_C(k)$ function does not depend upon α (in atomic units). These two differences can also be found for the corresponding electric fields which are determined as the gradients of the corresponding potentials. The $\mathbf{k}$-component (Fourier component) of the total electric filed (Coulomb + Uehling potentials) is $\mathbf{E_k} = -i\frac{4\pi}{k^2}(1 + U(k)) \cdot \mathbf{k}$, where the function $U(k)$ is

$$U(k) = \frac{1}{k\alpha^2}\left\{-\frac{10}{3} + \frac{8}{k^2\alpha^2} + \frac{1}{k^4\alpha^4}(k^4\alpha^4 + 2k^2\alpha^2 - 8)ln[1 + \frac{k^2\alpha^2}{2}]\right\} \tag{19}$$

and $\mathbf{k}$ is the wave vector. As follows from this formula each of the $\mathbf{E_k}$ components is oriented along the wave vector $\mathbf{k}$, i.e. the total electric field contains only the longitudinal components (there are no non-zero transverse components) and these components do not depend upon the time t.

IV. CONSECUTIVE APPROXIMATIONS UPON THE FINE STRUCTURE CONSTANT

In general, the short-range Uehling potential can be considered as a small correction to the Coulomb interparticle potential. The contributions of the Uehling potential can be taking into account with the use of the perturbation theory. The small parameter in this theory is the fine structure constant α (or the factor 2 α). Based on the existence of the radial O(2,1)-algebra for the original Coulomb two-body system (atom) we can find a very transparent physical sense for each order of approximation used in this procedure. Below in this Section, we restrict ourselves to the analysis of the Coulomb two-body systems. The cases of the Coulomb three- and four-body systems can be considered analogously. The Coulomb two-body system (or atom) includes the heavy nucleus with the electric charge Qe and electron with mass m_e and electric charge $-e$. The corresponding Schrödinger equation (in atomic units) takes the following form

$$\hat{H}\Psi = \left[-\frac{1}{2}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{L}^2}{r^2} - \frac{Q}{r}\right]\Psi = E\Psi \tag{20}$$

where $\hat{H}$ is the Hamiltonian, E is the energy of the system, $\hat{L}^2$ is the operator of the angular momentum of the system (atom) and Ψ is the wave function. The operator $\hat{L}^2$ depends only

upon two angular variables (Θ and ϕ) and it commutes with any operator which depends upon the radial variable r. The explicit form of the $\hat{L}^2$ operator is

$$\hat{L}^2 = -\Big[\frac{1}{\sin\Theta}\frac{\partial}{\partial\Theta}\Big(sin\Theta\frac{\partial}{\partial\Theta}\Big) + \frac{1}{\sin^2\Theta}\frac{\partial^2}{\partial\phi^2}\Big] \tag{21}$$

The eigenfunctions of the $\hat{L}^2$ operator are the spherical harmonics (see, e.g., [1]) $Y_{\ell m}(\Theta,\phi)$ and $\hat{L}^2 Y_{\ell m}(\Theta,\phi) = \ell(\ell+1)Y_{\ell m}(\Theta,\phi)$.

In [7] (see also [8] and [9]) it was shown that the three following operators

$$S = \frac{1}{2}r\Big(p_r^2 + \frac{\hat{L}^2}{r^2} + 1\Big) \quad , \quad T = rp_r \quad and \quad U = \frac{1}{2}r\Big(p_r^2 + \frac{\hat{L}^2}{r^2} - 1\Big) \tag{22}$$

form the non-compact O(2,1)-algebra with the commutation relations

$$[S,T] = -\imath U \quad , \quad [T,U] = \imath S \quad , \quad [U,S] = -\imath T \tag{23}$$

The Casimir operator of this algebra $C_2 = S^2 - U^2 - T^2$ equals to the $\hat{L}^2$ operator of the angular momentum. The exact coincidence of the Casimir operator C_2 of the radial algebra $O(2,1)$ with the Casimir operator $C_2 = L^2$ of the algebra of three-dimensional rotations $O(3)$ is related with the complementarity of the corresponding representations in the space of more general $Sp(6N,R)$-algebra representation (so-called Moshinsky complementarity of representations, see, e.g., [10]).

Based on this fact we can transform the operator $r(\hat{H} - E) = [(S+U) - E(S-U) + Q]$ from the Schrödinger equation by applying the unitary transformation $exp(\imath\beta T)$, where β is the real parameter and T is the generator from Eq.(22). Indeed, by using the well known Hausdorff formula

$$exp(-\imath\beta T)(S \pm U)exp(\imath\beta T) = exp(\pm\beta T)(S \pm U) \tag{24}$$

Now, we can chose $\beta = ln\sqrt{-2E}$ and reduce the original Schrödinger equation to the form

$$[\sqrt{-2E}S - Q]\phi(r,\Theta,\phi) = 0 \tag{25}$$

The operator S has the discrete spectrum [7], [11] which is written in the general form $S \mid n,\ell,m\rangle = n \mid n,\ell,m\rangle$, where $n = 1,2,3,\ldots$ is an integer positive number. From Eq.(25) one finds $E_n = -\frac{Q^2}{2n^2}$ (the energy spectrum in atomic units) and $\mid n,\ell,m\rangle = A\phi(r,\Theta,\phi)$, where A is an arbitrary numerical constant. All these facts and equations are very well known for the Coulomb two-body systems (atoms). It appears that we can modify our

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procedure for pure Coulomb systems to include the Uehling potential. Such a modification is discussed below.

First, we note that from Eq.(22) it follows that $r = S + U$. Second, the modified Uehling potential $rU(r)$ is written in the form:

$$rU(2br) = \frac{2\alpha Q}{3\pi}\left[\left(1 + \frac{b^2 r^2}{3}\right)K_0(2br) - \frac{br}{6}Ki_1(2br) - \left(\frac{b^2 r^2}{3} + \frac{5}{6}\right)Ki_2(2br)\right] \quad , \qquad (26)$$

This means that the Uehling potential is a function of the $2br = \frac{2}{\alpha}(S + U)$ variable. Such a variable contain the small dimensionless parameter (the fine structure constant) α. In Eq.(26) the parameter $\frac{2}{\alpha}$ plays the role of the cut-off parameter, since all modified Bessel functions $K_0(2br), Ki_1(2br)$ and $Ki_2(2br)$ decrease exponentially at large r. Briefly, this means that we can restrict the power series of the $rU(2br)$ potential to a very few first terms and expectation values of all these terms can be determined with the use of the commutation relations for the O(2,1)-algebra, Eq.(23). In particular, for me it was interesting to know that in the lowest order approximation the effect of vacuum polarisation can be represented as a small change of the electric charge (screening).

V. CUSP PROBLEM

As is well known in any Coulomb few-body system the expectation value of the following operator (in atomic units)

$$\hat{\nu}_{ij} = \frac{1}{\langle\delta(\mathbf{r}_{ij})\rangle}\delta(\mathbf{r}_{ij})\frac{\partial}{\partial r_{ij}} \qquad (27)$$

equals to the product of the corresponding electric charges q_1 and q_2. In particular, for the electron-nuclear Coulomb interaction written in atomic units te expectation value of the $\hat{\nu}_{eN}$ operator equals Q exactly. The operator, Eq.(27), has a great interest for the general theory of bound states in Coulomb few-body systems. On the other hand, the coincidence of the expectation value of this operator with its expected value, e.g., with Q, is often used in numerical computations to test the quality of trial wave functions.

Now, consider the case when Uehling potential is added to the Coulomb potential directly into the Schrödinger equation. This will lead to the change of the cusp condition between each pair of interacting particles. The fundamental problem is to find the $\nu_{ij} = \langle\hat{\nu}_{ij}\rangle$ value for few-body systems interacting by the potential which is the sum of Coulomb + Uehling

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potential. Formally, the answer can be written in the following form (in atomic units)

$$\nu_{ij} = q_i q_j \Big\{ 1 - \frac{\alpha}{3\pi} \big[\frac{5}{3} + 2\gamma - 2ln\alpha + 2lnr \big] \Big\} \tag{28}$$

where α is the fine structure constant, $\gamma \approx 0.577215\ldots$ is the Euler's constant. Note that the explicit expression for the ν_{ij} expectation value, Eq.(28), is $r-$dependent and its finite limit at $r \to 0$ does not exist. On the other hand, the correct definition of the cusp-value includes two-particle delta-function. For non-relativistic systems this delta-function is a constant at the distances shorter than $\Lambda_e = \alpha a_0 = \alpha$ (in atomic units), where Λ_e is the Compton wavelength. In general, the non-relativistic wave function cannot produce the actual electron density distribution at distances shorter than Λ_e. Instead it always gives the constant. Briefly, this means that we have to assume that $r = \alpha a_0 = \alpha$ in Eq.(28). Therefore, the cusp expectation value (or ν_{ij} value) is finite and its numerical value is

$$\nu_{ij} = q_i q_j \Big\{ 1 - \frac{\alpha}{3\pi} \big[\frac{5}{3} + 2\gamma \big] \Big\} \tag{29}$$

In other words, the Uehling potential produces a negative correction to the pure Coulomb cusp which is $\sim \alpha$. It will be very interesting to perform highly accurate computations for some few-body systems with the mixed interaction potential between electrically particles (Coulomb + Uehling). Then we can determine the expectation values of the actual electron-nuclear and electron-electron cusp values. Note that in modern highly accurate computations the cusp values are determined to the accuracy $\approx 1 \cdot 10^{-10} - 1 \cdot 10^{-12}$ $a.u.$ The expected Uehling correction to the pure Coulomb cusp is $\approx 1 \cdot 10^{-3}$ (or 0.1 %) and it can easily be detected in such computations.

VI. CONCLUSION

We have considered a number of properties of the Uehling potential. In particular, we have derived the expression for the lowest-order correction to the vacuum polarisation which contains the electron density distribution function $\rho(x)$ in atoms and/or in molecules. Such a representation has a number of advantages in various applications, including actual calculations of the vacuum polarisation in the mixed atomic states and variational procedures used to improve the electron density distribution function $\rho(x)$ from 'exact' QED-based Hamiltonians. We also derive the explicit expression for the Fourier spatial resolution of

the Uehling potential. It is shown that such a resolution contains only longitudinal waves of zero frequency. The formula for the Fourier spatial resolution of the Uehling potential is investigated. Small corrections produced by the short-range Uehling potential for actual Coulomb systems can be taking into account by a method based on the use of the non-trivial O(2,1)-group for the original Coulomb few-body systems. In conclusion, we wish to note that the Uehling potential has many other unique properties which were never investigated in earlier works, e.g., the 'corrected' cusp between two interacting electric charges. Some of these properties will be discussed in our future studies.

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